

Derivation of Master Equations in the Presence of Initial Correlations with Reservoir: Projection Method Revisited

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Abstract. We discuss the derivation of master equations in the presence of initial correlations with the reservoir. In van Hove's limit, the total system behaves as if it started from a factorized initial condition. A proper choice of Nakajima–Zwanzig's projection operator is crucial and the reservoir should be endowed with the mixing property.

1. Introduction

The derivation of master equations has been a central issue for decades in the field of quantum physics, both from a practical and fundamental point of view. The interests include dissipative dynamics in quantum optics [1, 2], understanding decoherence [3], the emergence of irreversibility [2, 4], and the influence of dissipation/decoherence on quantum information.

It is not a trivial problem how to describe the dissipative and irreversible dynamics of quantum systems, since the Schrödinger equation applies to closed systems and describes unitary evolutions. In the standard approach to this issue, one puts the system in a large reservoir to allow energy exchange and dissipation. Then, one applies the Schrödinger equation to the total (closed) system, system S+reservoir B, and extracts the dynamics of system S by tracing out the reservoir degrees of freedom,

$$\rho_S(t) = \text{tr}_B \rho(t), \quad (1)$$

which exhibits a non-unitary evolution and is described by a master equation. Here, $\rho(t)$ and $\rho_S(t)$ are the density operators of the total system and system S, respectively.

One of the targets of this article is to discuss a hypothesis that is taken for granted in most of such approaches: factorized (uncorrelated) initial conditions

$$\rho_0 = \rho_S \otimes \rho_B \quad (2)$$

are usually assumed in the derivation of master equations without any reasoning

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about the validity and the necessity of this hypothesis [1–4]. We will discuss in the following a derivation of master equations for generic (correlated) initial states. The reconsideration of the factorized initial condition (2) raises another question in the application of Nakajima–Zwanzig’s projection operator \mathcal{P} [2, 4–6], defined by the mapping

$$\rho(t) \longrightarrow \mathcal{P}\rho(t) = \text{tr}_B\{\rho(t)\} \otimes \Omega_B. \quad (3)$$

Which state of reservoir B should be taken as the reference state Ω_B of the projector \mathcal{P} ? We address these points and show the derivation of master equations in the presence of initial correlations. We clarify that the choice of \mathcal{P} is crucial and the reference state Ω_B should be endowed with the mixing property [7].

2. Framework

Let the total system consist of a small system S and a large reservoir B. The Hamiltonian of the total system reads

$$H = H_0 + \lambda H_{SB} = H_S + H_B + \lambda H_{SB}, \quad (4)$$

where H_S , H_B , and H_{SB} are the Hamiltonians of system S, reservoir B, and the interaction between them, respectively, and λ is the coupling constant. The corresponding Liouvillians are defined as the commutators with the Hamiltonians,

$$\mathcal{L} = -i[H, \cdot] = \mathcal{L}_0 + \lambda \mathcal{L}_{SB} = \mathcal{L}_S + \mathcal{L}_B + \lambda \mathcal{L}_{SB}. \quad (5)$$

Clearly,

$$[\mathcal{L}_S, \mathcal{L}_B] = 0. \quad (6)$$

We assume that the system Hamiltonian H_S admits a pure point spectrum, and the system Liouvillian \mathcal{L}_S is resolved in terms of its eigenprojections \tilde{Q}_m ,

$$\mathcal{L}_S = -i \sum_m \omega_m \tilde{Q}_m, \quad \sum_m \tilde{Q}_m = 1, \quad \tilde{Q}_m \tilde{Q}_n = \delta_{mn} \tilde{Q}_m. \quad (7)$$

In this article, we discuss the derivation of master equations via Nakajima–Zwanzig’s projection method, to implement the trace over the reservoir (1). We define two projection operators: \mathcal{P} defined by (3) and

$$\mathcal{Q} = 1 - \mathcal{P}. \quad (8)$$

They are projection operators since they satisfy

$$\mathcal{P} + \mathcal{Q} = 1, \quad \mathcal{P}^2 = \mathcal{P}, \quad \mathcal{Q}^2 = \mathcal{Q}, \quad \mathcal{P}\mathcal{Q} = \mathcal{Q}\mathcal{P} = 0, \quad (9)$$

assuming the normalization of the reference state $\text{tr}_B \Omega_B = 1$. One of the main issues of the present article is to discuss the choice of the reference state Ω_B . We

do not know at this moment which state should be taken as the reference state Ω_B . We only assume its stationarity here, $\mathcal{L}_B \Omega_B = 0$, and will specify other features later.

Notice that

$$[\mathcal{P}, \mathcal{L}_S] = 0, \quad [\mathcal{Q}, \mathcal{L}_S] = 0, \quad \mathcal{P}\mathcal{L}_B = \mathcal{L}_B\mathcal{P} = 0, \quad \mathcal{Q}\mathcal{L}_B = \mathcal{L}_B\mathcal{Q} = \mathcal{L}_B, \quad (10)$$

and that we can always accomplish

$$\mathcal{P}\mathcal{L}_{SB}\mathcal{P} = 0, \quad (11)$$

by redefining the Hamiltonians H_S and H_{SB} .

3. Projection Method

Let us now start the derivation of the master equation for $\rho_S(t)$ defined by (1). Consider the initial-value problem for the total system,

$$\frac{d}{dt}\rho(t) = \mathcal{L}\rho(t), \quad \rho(0) = \rho_0, \quad (12)$$

where the initial density operator ρ_0 is *not* assumed to be factorized like (2). By projecting the Liouville equation (12) onto the two subspaces defined by \mathcal{P} and \mathcal{Q} , and noting the properties (10) and (11), one gets

$$\frac{d}{dt}\mathcal{P}\rho = \mathcal{L}_S\mathcal{P}\rho + \lambda\mathcal{P}\mathcal{L}_{SB}\mathcal{Q}\rho, \quad (13a)$$

$$\frac{d}{dt}\mathcal{Q}\rho = \mathcal{L}'_0\mathcal{Q}\rho + \lambda\mathcal{Q}\mathcal{L}_{SB}\mathcal{P}\rho, \quad (13b)$$

respectively, where

$$\mathcal{L}'_0 = \mathcal{L}_0 + \lambda\mathcal{Q}\mathcal{L}_{SB}\mathcal{Q}. \quad (14)$$

By formally integrating out the second equation and plugging the result into the first, one gets the following equation for the \mathcal{P} -projected operator in the interaction picture [6],

$$\frac{d}{dt}e^{-\mathcal{L}_S t}\mathcal{P}\rho(t) = \lambda^2 \int_0^t dt' e^{-\mathcal{L}_S t}\mathcal{P}\mathcal{L}_{SB}e^{\mathcal{L}'_0(t-t')}\mathcal{L}_{SB}\mathcal{P}\rho(t') + \lambda e^{-\mathcal{L}_S t}\mathcal{P}\mathcal{L}_{SB}e^{\mathcal{L}'_0 t}\mathcal{Q}\rho_0. \quad (15)$$

This is an *exact* and *non-Markovian* master equation since the first term on the right-hand side contains a memory integral. The last term, on the other hand, represents the contribution arising from a possible initial correlation between system S and reservoir B. In fact, this term is absent when the initial state ρ_0 is factorized like (2) and the reference state of the projector is accordingly chosen as $\Omega_B = \rho_B$. We are interested in the fate of this inhomogeneous term in the following arguments, when there is an initial correlation between system S and reservoir B.

4. Van Hove's Limit

Let us make the Markovian approximation here, since the exact master equation (15) is usually too complicated to handle for general systems and the Markovian approximation is valid for various practical situations. In this article, we apply van Hove's limit [8] for this purpose. That is, we take the weak-coupling limit $\lambda \rightarrow 0$ and the long-time limit $t \rightarrow \infty$ at the same time, keeping the scaled time $\tau = \lambda^2 t$ finite. This rescaling in time eliminates the memory, and the system exhibits a Markovian dynamics in the scaled time τ .

Now consider the density operator

$$\rho_I^{(\lambda)}(\tau) = e^{-\mathcal{L}_S \tau / \lambda^2} \mathcal{P} \rho(\tau / \lambda^2), \quad (16)$$

that satisfies, for any nonvanishing λ ,

$$\begin{aligned} \frac{d}{d\tau} \rho_I^{(\lambda)}(\tau) = & \int_0^{\tau/\lambda^2} dt e^{-\mathcal{L}_S \tau / \lambda^2} \mathcal{P} \mathcal{L}_{\text{SB}} e^{\mathcal{L}'_0(\tau/\lambda^2 - t)} \mathcal{L}_{\text{SB}} \mathcal{P} e^{\mathcal{L}_S t} \rho_I^{(\lambda)}(\lambda^2 t) \\ & + \frac{1}{\lambda} e^{-\mathcal{L}_S \tau / \lambda^2} \mathcal{P} \mathcal{L}_{\text{SB}} e^{\mathcal{L}'_0 \tau / \lambda^2} \mathcal{Q} \rho_0, \end{aligned} \quad (17)$$

with the initial condition

$$\rho_I^{(\lambda)}(0) = \mathcal{P} \rho_0. \quad (18)$$

By integrating (17), one gets

$$\begin{aligned} \rho_I^{(\lambda)}(\tau) = & \mathcal{P} \rho_0 + \int_0^\tau d\tau' \int_0^{\tau'/\lambda^2} dt e^{-\mathcal{L}_S \tau' / \lambda^2} \mathcal{P} \mathcal{L}_{\text{SB}} e^{\mathcal{L}'_0(\tau'/\lambda^2 - t)} \mathcal{L}_{\text{SB}} \mathcal{P} e^{\mathcal{L}_S t} \rho_I^{(\lambda)}(\lambda^2 t) \\ & + \frac{1}{\lambda} \int_0^\tau d\tau' e^{-\mathcal{L}_S \tau' / \lambda^2} \mathcal{P} \mathcal{L}_{\text{SB}} e^{\mathcal{L}'_0 \tau' / \lambda^2} \mathcal{Q} \rho_0, \end{aligned} \quad (19)$$

which is arranged into the form [7]

$$\rho_I^{(\lambda)}(\tau) = \mathcal{P} \rho_0 + \sum_{m,n} \int_0^\tau d\tau' e^{i(\omega_m - \omega_n)\tau' / \lambda^2} \mathcal{K}_{mn}^{(\lambda)}(\tau - \tau') \rho_I^{(\lambda)}(\tau') + \mathcal{I}^{(\lambda)}(\tau), \quad (20)$$

where

$$\mathcal{K}_{mn}^{(\lambda)}(\tau) = \mathcal{P} \tilde{\mathcal{Q}}_m \mathcal{L}_{\text{SB}} \mathcal{R}_m^{(\lambda)}(\tau) \mathcal{L}_{\text{SB}} \tilde{\mathcal{Q}}_n \mathcal{P}, \quad (21a)$$

$$\mathcal{I}^{(\lambda)}(\tau) = \lambda \sum_m \mathcal{P} \tilde{\mathcal{Q}}_m \mathcal{L}_{\text{SB}} \mathcal{R}_m^{(\lambda)}(\tau) \mathcal{Q} \rho_0. \quad (21b)$$

The important feature is that the kernel $\mathcal{K}_{mn}^{(\lambda)}(\tau)$ and the contribution of the initial correlation $\mathcal{I}^{(\lambda)}(\tau)$ are both governed by the operator

$$\mathcal{R}_m^{(\lambda)}(\tau) = \int_0^{\tau/\lambda^2} dt \mathcal{Q} e^{(\mathcal{L}'_0 + i\omega_m)t}. \quad (22)$$

Therefore, the van Hove limit of this key operator $\mathcal{R}_m^{(\lambda)}(\tau)$ completes the van Hove limit of the master equation (20).

5. Main Theorem

As we will see later, the van Hove limit of $\mathcal{R}_m^{(\lambda)}(\tau)$ results in

$$\mathcal{R}_m^{(\lambda)}(\tau) \xrightarrow{\lambda \rightarrow 0} -\frac{\mathcal{Q}}{\mathcal{L}_0 + i\omega_m - 0^+} \quad (\tau > 0), \quad (23)$$

and it immediately leads us to the conclusion that, in van Hove's limit, the memory kernel $\mathcal{K}_{mn}^{(\lambda)}(\tau)$ in (21a) is reduced to a Markovian generator

$$\mathcal{K}_{mn}^{(\lambda)}(\tau) \xrightarrow{\lambda \rightarrow 0} \mathcal{K}_{mn}^{(0)} = -\mathcal{P}\tilde{Q}_m\mathcal{L}_{\text{SB}}\frac{\mathcal{Q}}{\mathcal{L}_0 + i\omega_m - 0^+}\mathcal{L}_{\text{SB}}\tilde{Q}_n\mathcal{P}, \quad (24)$$

while the correlation term $\mathcal{I}^{(\lambda)}(\tau)$ in (21b) disappears

$$\mathcal{I}^{(\lambda)}(\tau) \xrightarrow{\lambda \rightarrow 0} 0, \quad (25)$$

so that the reduced dynamics (20) becomes

$$\rho_{\text{I}}^{(\lambda)}(\tau) \xrightarrow{\lambda \rightarrow 0} \mathcal{P}\rho_0 + \sum_{m,n} \int_0^\tau d\tau' \delta_{mn} \mathcal{K}_{mn}^{(0)} \rho_{\text{I}}(\tau') = \mathcal{P}\rho_0 + \int_0^\tau d\tau' \mathcal{K} \rho_{\text{I}}(\tau'). \quad (26)$$

The master equation in van Hove's limit reads therefore

$$\frac{d}{d\tau} \rho_{\text{I}}(\tau) = \mathcal{K} \rho_{\text{I}}(\tau), \quad \mathcal{K} = \sum_m \mathcal{K}_{mm}^{(0)} = -\sum_m \mathcal{P}\tilde{Q}_m\mathcal{L}_{\text{SB}}\frac{\mathcal{Q}}{\mathcal{L}_0 + i\omega_m - 0^+}\mathcal{L}_{\text{SB}}\tilde{Q}_m\mathcal{P}, \quad (27a)$$

with the initial condition

$$\rho_{\text{I}}(0) = \mathcal{P}\rho_0 = \text{tr}_{\text{B}}\{\rho_0\} \otimes \Omega_{\text{B}}. \quad (27b)$$

That is, even if the initial state ρ_0 is not in a factorized form, but rather there is entanglement, or simply a classical correlation, between system S and reservoir B, all correlations disappear in van Hove's limit and system S behaves as if the total system started from the factorized initial state (27b) with a reservoir state Ω_{B} specified below.

The key formula (23), and therefore the master equation (27) in van Hove's limit, are proved under the following assumptions:

- (i) the initial (correlated) state of the total system, ρ_0 , belongs to a single sector.
That is, ρ_0 is given in the form

$$\rho_0 = \sum_i L_i (1_{\text{S}} \otimes \Omega_{\text{B}}) L_i^\dagger, \quad (28)$$

where $1_S \otimes \Omega_B$ is the state which specifies the sector and L_i 's are bounded operators;

- (ii) the state Ω_B is mixing, and therefore the reservoir Liouvillian \mathcal{L}_B bears a simple eigenvalue 0. We assume in addition that the remaining part of the spectrum of \mathcal{L}_B is absolutely continuous;
- (iii) the projection operator \mathcal{P} adopted in (23) and (27) must be defined in terms of Ω_B that is mixing and “contained” in the initial state ρ_0 of the form (28).

6. Mixing

The state Ω_B is called mixing with respect to the reservoir dynamics $e^{\mathcal{L}_B t}$ iff

$$\text{tr}_B\{X(t)Y\Omega_B\} = \text{tr}_B\{Xe^{\mathcal{L}_B t}Y\Omega_B\} \xrightarrow{t \rightarrow \infty} \text{tr}_B\{X\Omega_B\} \text{tr}_B\{Y\Omega_B\} \quad (29)$$

for any bounded superoperators X and Y of the reservoir B, where $X(t) = e^{-\mathcal{L}_B t} X e^{\mathcal{L}_B t}$ [9]. One of the typical mixing states is the thermal equilibrium state of bosons at finite temperature $\Omega_B \sim e^{-\beta H_B}$ [7], which often appears in the literature. Among other interesting mixing states, there are nonequilibrium steady states, where system B consists of two reservoirs with different temperatures and steady current flows between them. Such a situation is also within our scope.

Note here that a state ρ_0 that refers [in the sense of (28)] to two (or more) different mixing states of an infinite reservoir cannot be a physical state, since it is the superposition of states belonging to different inequivalent sectors. (Imagine, for example, the superposition of states with different temperatures.) Hypothesis (i) is therefore reasonable from this point of view.

The important consequence of mixing is that it implies the existence of the point spectrum 0 of \mathcal{L}_B [9]. Let us consider the time evolution, driven by the reservoir free Liouvillian \mathcal{L}_B , of the expectation value of any operator $D = \sum_j A_j \otimes X_j$, starting from the initial state ρ_0 of the kind (28), where A_j 's are operators of system S and X_j 's bounded operators of reservoir B. Then, the mixing property (29) of Ω_B yields

$$\begin{aligned} \text{tr}\{De^{\mathcal{L}_B t}\rho_0\} &= \sum_i \sum_j \text{tr}_B[X_j e^{\mathcal{L}_B t} \text{tr}_S\{A_j L_i(1_S \otimes \Omega_B)L_i^\dagger\}] \\ &\xrightarrow{t \rightarrow \infty} \sum_i \sum_j \text{tr}_B\{X_j \Omega_B\} \text{tr}\{A_j L_i(1_S \otimes \Omega_B)L_i^\dagger\} = \text{tr}[D(\text{tr}_B\{\rho\} \otimes \Omega_B)], \end{aligned} \quad (30)$$

and in this sense, we have

$$e^{\mathcal{L}_B t}\rho_0 \xrightarrow{t \rightarrow \infty} \text{tr}_B\{\rho_0\} \otimes \Omega_B \quad (31)$$

for any state ρ_0 belonging to the sector of $1_S \otimes \Omega_B$. This shows that \mathcal{L}_B bears one and the only simple eigenvalue (in the relevant sector), which is 0. It is essential

to note that, if \mathcal{L}_B admits more simple eigenvalues, such as for an ergodic state Ω_B [9], it is not possible to derive a master equation as we will see later. Recall further that mixing does not exclude a singular continuous spectrum, as far as it is transient, i.e., Riemann–Lebesgue’s lemma holds [9]. Hypothesis (ii) therefore assumes stronger conditions than mixing.

Finally, Eq. (31) also shows that the eigenprojection Π_0 belonging to the simple eigenvalue 0,

$$\mathcal{L}_B \Pi_0 = \Pi_0 \mathcal{L}_B = 0, \quad (32)$$

acts on the state ρ in the relevant sector as

$$\Pi_0 \rho = \text{tr}_B\{\rho\} \otimes \Omega_B. \quad (33)$$

The projector \mathcal{P} suggested in Hypothesis (iii) is nothing but this eigenprojection Π_0 : the proper choice of the projector is

$$\mathcal{P} = \Pi_0, \quad (34)$$

where the reference state Ω_B should be endowed with the mixing property and contained in the initial state as (28). A wrong projector yields secular terms and prevents us from deriving a master equation, as we will see in the next section.

7. The Key Formula

Let us finally prove the key formula (23) with the projector (34). It requires a few steps, since the spectral property of \mathcal{L}'_0 given in (14) is not known. We start by noting that $\mathcal{Q}e^{\mathcal{L}'_0 t} = \mathcal{Q}e^{\mathcal{L}t}\mathcal{Q}$ and hence $\|\mathcal{Q}e^{\mathcal{L}'_0 t}\| = \|\mathcal{Q}e^{\mathcal{L}t}\mathcal{Q}\| \leq \|\mathcal{Q}\|^2 \cdot \|e^{\mathcal{L}t}\| = 1$. One therefore obtains

$$\lambda^n \mathcal{R}_m^{(\lambda)}(\tau) = \lambda^n \int_0^{\tau/\lambda^2} dt \mathcal{Q}e^{(\mathcal{L}'_0 + i\omega_m)t} \rightarrow 0 \quad \text{as } \lambda \rightarrow 0 \quad (n > 2) \quad (35)$$

in van Hove’s limit, irrespective of the spectrum of \mathcal{L}'_0 .

Second, the convolution

$$\int_0^t dt' e^{\mathcal{L}_0(t-t')} \mathcal{Q} \mathcal{L}_{SB} \mathcal{Q} e^{\mathcal{L}'_0 t'} \quad (36)$$

is bounded for any t , *provided the projector is properly chosen as $\mathcal{P} = \Pi_0$ and the point spectrum of \mathcal{L}_0 is removed by the projection $\mathcal{Q} = 1 - \Pi_0$* . See Ref. [7].

Now, by using

$$e^{\mathcal{L}'_0 t} = e^{\mathcal{L}_0 t} + \lambda \int_0^t dt' e^{\mathcal{L}_0(t-t')} \mathcal{Q} \mathcal{L}_{SB} \mathcal{Q} e^{\mathcal{L}'_0 t'}, \quad (37)$$

we expand the relevant quantity (22) as

$$\mathcal{R}_m^{(\lambda)}(\tau) = \int_0^{\tau/\lambda^2} dt \mathcal{Q} e^{(\mathcal{L}_0 + i\omega_m)t} + \lambda \int_0^{\tau/\lambda^2} dt \int_0^t dt' e^{(\mathcal{L}_0 + i\omega_m)t} e^{-\mathcal{L}_0 t'} \mathcal{Q} \mathcal{L}_{\text{SB}} \mathcal{Q} e^{\mathcal{L}'_0 t'}. \quad (38)$$

Let us split the first term into two contributions, the discrete and the continuous spectra of \mathcal{L}_0 , by the projection operators Π_0 and $1 - \Pi_0$. For $\tau > 0$, one gets

$$\begin{aligned} & \int_0^{\tau/\lambda^2} dt \mathcal{Q} e^{(\mathcal{L}_0 + i\omega_m)t} \\ &= \int_0^{\tau/\lambda^2} dt \mathcal{Q} \Pi_0 e^{(\mathcal{L}_0 + i\omega_m)t} + \int_0^{\tau/\lambda^2} dt \mathcal{Q} (1 - \Pi_0) e^{(\mathcal{L}_0 + i\omega_m)t} \\ &= \frac{\tau}{\lambda^2} \mathcal{Q} \Pi_0 \tilde{Q}_m + \sum_{n \neq m} \mathcal{Q} \Pi_0 \tilde{Q}_n \frac{e^{i(\omega_m - \omega_n)\tau/\lambda^2} - 1}{i(\omega_m - \omega_n)} + \mathcal{Q} (1 - \Pi_0) \frac{e^{(\mathcal{L}_0 + i\omega_m)\tau/\lambda^2} - 1}{\mathcal{L}_0 + i\omega_m - 0^+}, \end{aligned} \quad (39)$$

which shows that the only possible divergence of the relevant operator in (22) in van Hove's limit $\lambda \rightarrow 0$ comes from the point spectrum of \mathcal{L}_0 (i.e. the first term of the last expression). If $\mathcal{P} = \Pi_0$, however, the divergent term disappears due to $\mathcal{Q} \Pi_0 = 0$: the contributions of the point spectrum are properly removed by $\mathcal{Q} = 1 - \Pi_0$. The correct projection operator $\mathcal{P} = \Pi_0$ allows us to arrange the second term in (38) into

$$\begin{aligned} & \lambda \int_0^{\tau/\lambda^2} dt \int_0^t dt' e^{(\mathcal{L}_0 + i\omega_m)t} e^{-\mathcal{L}_0 t'} \mathcal{Q} \mathcal{L}_{\text{SB}} \mathcal{Q} e^{\mathcal{L}'_0 t'} \\ &= \lambda \frac{\mathcal{Q}}{\mathcal{L}_0 + i\omega_m - 0^+} e^{i\omega_m \tau/\lambda^2} \int_0^{\tau/\lambda^2} dt e^{\mathcal{L}_0(\tau/\lambda^2 - t)} \mathcal{Q} \mathcal{L}_{\text{SB}} \mathcal{Q} e^{\mathcal{L}'_0 t} \\ &\quad - \lambda \frac{\mathcal{Q}}{\mathcal{L}_0 + i\omega_m - 0^+} \mathcal{L}_{\text{SB}} \int_0^{\tau/\lambda^2} dt \mathcal{Q} e^{(\mathcal{L}'_0 + i\omega_m)t}, \end{aligned} \quad (40)$$

and we arrive at the recurrence formula

$$\begin{aligned} \mathcal{R}_m^{(\lambda)}(\tau) &= \mathcal{Q} \frac{e^{(\mathcal{L}_0 + i\omega_m)\tau/\lambda^2} - 1}{\mathcal{L}_0 + i\omega_m - 0^+} \\ &\quad + \lambda \frac{\mathcal{Q}}{\mathcal{L}_0 + i\omega_m - 0^+} e^{i\omega_m \tau/\lambda^2} \int_0^{\tau/\lambda^2} dt e^{\mathcal{L}_0(\tau/\lambda^2 - t)} \mathcal{Q} \mathcal{L}_{\text{SB}} \mathcal{Q} e^{\mathcal{L}'_0 t} \\ &\quad - \lambda \frac{\mathcal{Q}}{\mathcal{L}_0 + i\omega_m - 0^+} \mathcal{L}_{\text{SB}} \mathcal{R}_m^{(\lambda)}(\tau) \quad (\tau > 0). \end{aligned} \quad (41)$$

The integral in the second term is the convolution (36), which is bounded for $\tau/\lambda^2 \rightarrow \infty$ since the point spectrum of \mathcal{L}_0 is removed by the projection $\mathcal{Q} = 1 - \Pi_0$.

Therefore, by iterating the expansion (41) twice and by noting

$$\lim_{t \rightarrow \pm\infty} (1 - \Pi_0) \frac{e^{(\mathcal{L}_0 + i\omega_m)t}}{\mathcal{L}_0 + i\omega_m \mp 0^+} = 0 \quad (42)$$

together with (35), we derive the key formula (23).

In summary, the correct projector $\mathcal{P} = \Pi_0$ helps us to manage the subtle point spectrum 0 of \mathcal{L}_B . With a wrong projector, we would fail to appropriately remove it, Eq. (23) would not hold anymore, and $\mathcal{R}_m^{(\lambda)}(\tau)$ would diverge in van Hove's limit. This is because the wrong operator projects the reservoir onto a wrong state, so that the system evolution is frustrated, and develops secular terms in τ/λ^2 [like in Eq. (39)].

As stressed in Sec. 6, the reference state of the reservoir must be mixing in order that no discrete eigenvalue different from 0 exists. Otherwise, the point spectrum (except 0) is out of control, since we do not know the eigenprojections other than Π_0 , and again the emergence of secular terms is inevitable. Moreover, it should be noticed that the mixing property of the reservoir is crucial even for a *factorized* initial state like (2).

8. Concluding Remarks

In this article, we described the derivation of master equations via Nakajima–Zwanzig's projection operator method in the presence of the initial correlations with a reservoir. In van Hove's limit, the initial correlation disappears and the total system behaves as if it started from a factorized initial condition. It was demonstrated that (even for a factorized initial condition) the choice of the projection operator is crucial and a wrong projection provokes secular terms. The mixing property of the reservoir is essential to the derivation of master equations.

The factorization of the initial state in van Hove's limit implies that the total system is *factorized at any moment* in the scaled time τ , since the “initial time” $t = 0$ has no particular status. It is actually possible to prove it, i.e. [7]

$$\lim_{\lambda \rightarrow 0} \mathcal{Q}\rho(\tau/\lambda^2) = 0. \quad (43)$$

It is worth noting that the interaction between system S and reservoir B is not essential to the factorization: *free evolution eliminates the correlation, and the reservoir relaxes into the mixing state* Ω_B . Indeed, for any state ρ_0 of the total system of the type (28) with a mixing state Ω_B , we have

$$e^{\mathcal{L}_0 t} \rho_0 \xrightarrow{t \rightarrow \infty} e^{\mathcal{L}_S t} \Pi_0 \rho_0 = e^{\mathcal{L}_S t} \text{tr}_B \{\rho_0\} \otimes \Omega_B, \quad (44)$$

where the contribution of the continuous spectrum decays out due to the mixing property. [See Eq. (31).] In the rescaled time τ , the factorization is very rapid

(order λ^2 in the scaled time τ), and the total system looks factorized at any moment. The timescales of the factorization and the mixing are related not only to the spread of the initial correlation and the perturbation from the mixing state but also to the size of the relevant reservoir observables. These issues are discussed in detail in Ref. [7].

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